MULT.EU.SIM

« European Multiscale Simulation for the Computational Era »

"MULT.EU.SIM will provide the European Commission with a constructed case allowing it to decide whether or not to launch a proactive initiative in the field of multiscale modelling and simulation for nanoelectronics."

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A JOINT VISION ON THE PERSPECTIVES OF MULTISCALE MODELLING AND SIMULATION FOR NANODEVICES

Where do we stand?

The last years have seen the emergence of a broad array of novel products based on components structured at the nanoscale. The design of such systems spanning a wide range of length- and time-scales requires models based on realistic descriptions of the nanoscale building blocks. Integrating the quantum effects that dominate at the nanoscale into these models should be easily feasible as ab initio methods are well developed in Europe. However, the larger scales of nanodevices, the evolution of a system consisting of millions of atoms as a whole, cannot be cannot be predicted by means of ab initio. On each length- and time-scale, specific phenomena arise which cannot be described realistically but on their own level of detail. Not all interaction must necessarily be treated within the first principles framework. To succeed in describing the whole nanodevices in their complexity, a hierarchy of level of treatment must be introduced in which ab initio would be treated only as a subsystem, in order to extract relevant information to complete the upper-level model for the full system. A modelling and simulation "toolbox" is therefore called for, combining several models in a multiscale realistic and comprehensive description. Yet, despite much research in this direction, there a few demonstrated examples to date, which address present day R&D requirements of the European industry and research community.

What are we aiming at?

The goal is to achieve integrated modelling suites for nanodevices, bridging across the different scales from first principles to industrial application. The creation of a realistic and comprehensive simulation capability will allow the design of new devices bypassing most of the fabrication test runs, thereby accelerating the pace of development while in the same time sharply reducing the costs (time and money wise), and consequently gaining in competitiveness. Ultimately, the availability of such multiscale methods will put Europe's industry in a strong IPR position.

Those assessments are supported by a strong consensus of the simulation community, stemming from various contributions as well as from a survey conducted by the MULT.EU.SIM consortium. The conclusion of this survey is that multiscale simulation has great potential impact on S&T future progress, provided the (strategic) means of realizing it are given. In addition, the development of key enabling technologies (KETs) such as nanoelectronics, and thus the promotion of design capabilities, have been outlined as priorities in the EU technological strategy.

How do we get there?

This European vision will serve as the foundation for a joint effort in a field that is currently very fragmented. The development of multiscale simulation requires first furthering and optimizing the computational resources. Besides increasing the capacity to the petaflop or even the exaflop, it means supporting the progress in codes, theory and numerical algorithms, as these progresses contribute as well to the improvement of the effective computational power. The existing software tools need to be integrated in the multiscale strategy and adapted to reusability and modularity. Conceiving those new design tools implies a strong collaboration across disciplines and between academia and industry. A data-sharing system is notably called for, allowing researchers to use a broader set of information, and ultimately render more accurate models. In addition, empirical testing is still required to complement the computational methods, providing data to validate the key results and fill in the gaps. In the end, collaboration on creating new tools will rapidly increase the pace of innovation. Lastly, this foreseen integrated environment calls for an overall coordination effort (running along the specific projects and housing the transverse numerical effort), of which means the European Commission could be the supplier.